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What is hidden behind a phase diagram?

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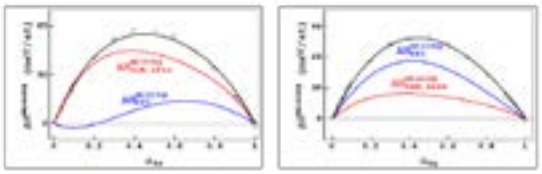
The thermodynamics of binary alloys is still far from being well understood despite numerous studies, in particular when the two constituents have very different atomic volumes. That is the case for the Au-Ni and Ag-Cu alloys that tend to phase separate and possess a large size mismatch. The phase diagrams of the two systems are characterized by a large miscibility gap. This apparent simplicity is, nevertheless, undermined by studies on the local order (short-range-order SRO). The ordering SRO observed experimentally is agreement with the phase diagram for Ag-Cu whereas it remains controversial for Au-Ni. We present a novel energetic model that takes into account atomistic relaxations to describe the thermodynamic properties of binary alloys . It involves of the calculation of site energies in a relaxed random solid solution as a function of the local composition and of the nominal concentration. The numerical results are obtained using N-body interatomic potentials derived on the second moment approximation (SMA) of the tight-binding scheme. This new model allows us to determine the effective pair interactions (EPI) that drive the SRO and to evaluate their contribution to the mixing enthalpy, as well as that of related to the lattice mismatch between the components. We apply this formalism to the Au-Ni and Ag-Cu alloys. Monte Carlo (MC) simulations on rigid lattice using this energetic model lead to phase diagrams that are in remarkable agreement with that obtained with SMA-MC simulations and the experimental ones. We show that the phase separation is mainly driven by the elastic contribution for Au-Ni and by the EPI's contribution for Ag-Cu. Furthermore for Au-Ni, SRO which are related to the EPIs, display a sign change as a function of the concentration.



Biography

Fabienne Berthier completed her education from Engineering School at Grenoble in Materials and Electrochemistry, 1982-1985. Her research interests include Atomistic simulations, multiscale modelling, thermodynamic properties of alloy at interfaces (surfaces, grain boundaries) and nanoalloys, aging kinetics. Her expertise is in modeling the thermodynamical properties of alloys to predict phase diagrams. She has developed a methodology that mixes a rigid lattice using model with off lattice Monte Carlo simulations. This mixed approach is very efficient to predict and analyze the interfacial segregation as for example at grain boundaries, surfaces and nanoparticles. She has also an expertise in Growth Kinetics and Ageing Kinetics.

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